



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 08:13 pm BST

PDB ID : 6HXW
Title : structure of human CD73 in complex with antibody IPH53
Authors : Roussel, A.; Amigues, B.
Deposited on : 2018-10-18
Resolution : 2.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

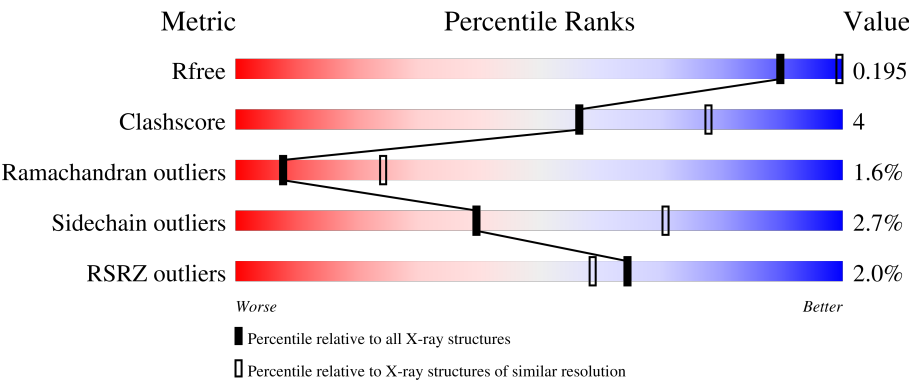
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	<div><div>89%9%</div></div>
1	B	527	<div><div>90%9%</div></div>
2	C	231	<div><div>2%80%13%7%</div></div>
2	H	231	<div><div>6%81%11%7%</div></div>
3	D	209	<div><div>85%13%</div></div>

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Mol	Chain	Length	Quality of chain
3	L	209	<div><div></div><div>3%</div><div>78%</div><div>18%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15507 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4074	2588	700	767	19			
1	B	523	Total	C	N	O	S	0	0	0
			4071	2587	700	765	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	HIS	PHE	conflict	UNP P21589
A	549	HIS	SER	conflict	UNP P21589
A	550	HIS	THR	conflict	UNP P21589
A	551	HIS	GLY	conflict	UNP P21589
A	552	HIS	SER	conflict	UNP P21589
B	548	HIS	PHE	conflict	UNP P21589
B	549	HIS	SER	conflict	UNP P21589
B	550	HIS	THR	conflict	UNP P21589
B	551	HIS	GLY	conflict	UNP P21589
B	552	HIS	SER	conflict	UNP P21589

- Molecule 2 is a protein called IPH53 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	215	Total	C	N	O	S	698	0	0
			1642	1044	276	316	6			
2	H	215	Total	C	N	O	S	0	0	0
			1642	1044	276	316	6			

- Molecule 3 is a protein called IPH53 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	209	Total	C	N	O	S	816	0	0
			1618	1015	269	329	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1618	1015	269	329	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	229	Total	O	0	0
			229	229		

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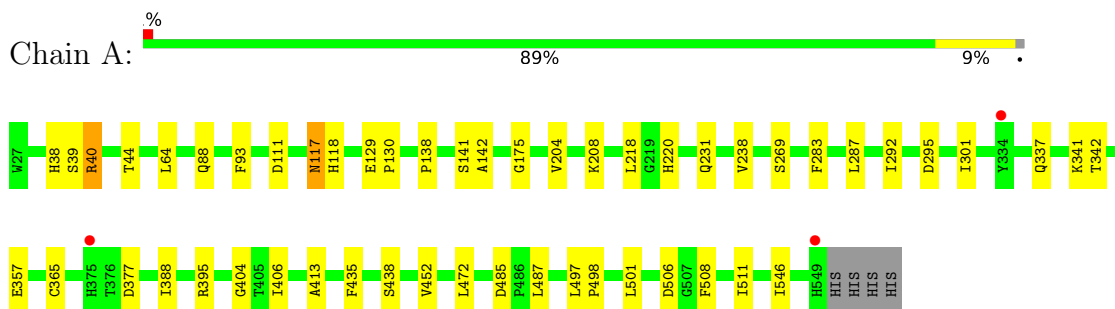
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	273	Total 273	O 273	0	0
6	C	62	Total 62	O 62	0	0
6	D	66	Total 66	O 66	0	0
6	H	93	Total 93	O 93	0	0
6	L	87	Total 87	O 87	0	0

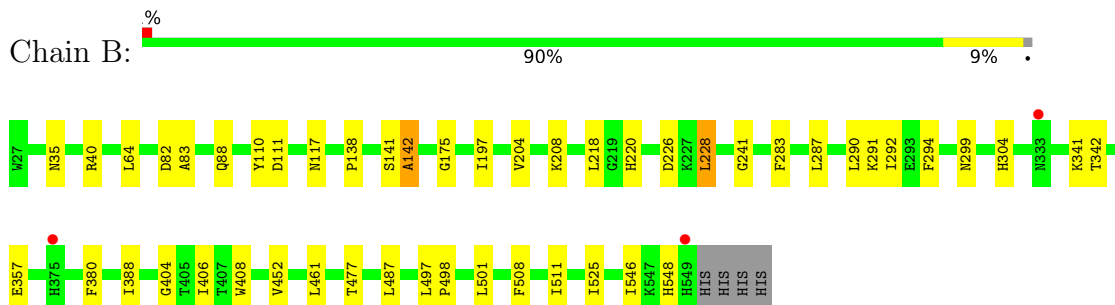
3 Residue-property plots

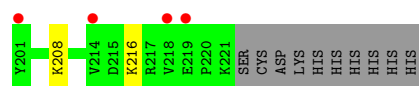
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5'-nucleotidase

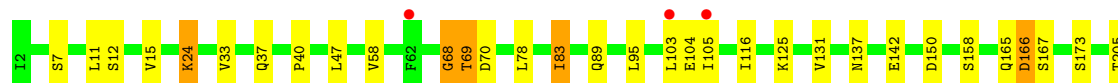
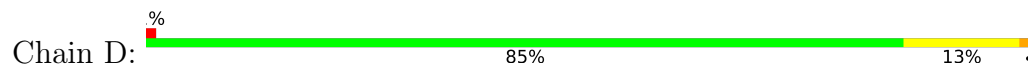


- Molecule 1: 5'-nucleotidase

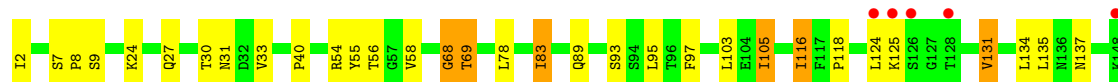
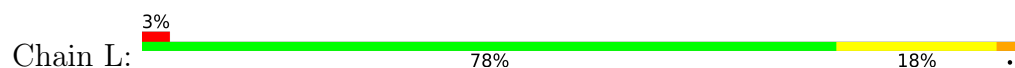




• Molecule 3: IPH53 light chain



• Molecule 3: IPH53 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	195.35Å 209.43Å 65.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 2.78 48.84 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.84-2.78) 99.5 (48.84-2.78)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.192 , 0.232 0.193 , 0.195	Depositor DCC
R_{free} test set	3773 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15507	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/4161	0.73	0/5639
1	B	0.52	0/4158	0.72	0/5635
2	C	0.44	0/1685	0.72	0/2295
2	H	0.47	0/1685	0.70	0/2295
3	D	0.43	0/1653	0.75	1/2245 (0.0%)
3	L	0.46	0/1653	0.78	1/2245 (0.0%)
All	All	0.48	0/14995	0.73	2/20354 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	7	SER	N-CA-C	-5.45	96.28	111.00
3	D	7	SER	N-CA-C	-5.13	97.16	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	0	4037	32	0
1	B	4071	0	4029	31	0
2	C	1642	0	1601	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1642	0	1601	10	0
3	D	1618	0	1570	13	0
3	L	1618	0	1570	23	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	229	0	0	1	0
6	B	273	0	0	0	0
6	C	62	0	0	1	0
6	D	66	0	0	0	0
6	H	93	0	0	0	0
6	L	87	0	0	0	0
All	All	15507	0	14434	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:89:GLN:HE21	3:D:95:LEU:HD11	1.22	1.03
3:D:24:LYS:HE2	3:D:70:ASP:OD1	1.62	0.99
3:L:116:ILE:HD11	3:L:193:CYS:HB3	1.49	0.93
1:A:388:ILE:HG13	1:A:497:LEU:HD13	1.53	0.90
3:L:30:THR:HG22	3:L:31:ASN:H	1.35	0.90
1:B:388:ILE:HG13	1:B:497:LEU:HD13	1.53	0.90
1:A:497:LEU:HD12	1:A:498:PRO:HD2	1.53	0.90
1:B:497:LEU:HD12	1:B:498:PRO:HD2	1.56	0.88
3:D:89:GLN:NE2	3:D:95:LEU:HD11	1.90	0.84
1:A:295:ASP:HB3	1:A:301:ILE:HD11	1.67	0.76
1:A:40:ARG:HG3	1:A:44:THR:HG21	1.69	0.75
3:L:116:ILE:HD13	3:L:206:LYS:HB3	1.70	0.73
1:B:141:SER:O	1:B:142:ALA:HB3	1.89	0.72
3:L:30:THR:CG2	3:L:31:ASN:H	2.06	0.69
1:A:238:VAL:HG21	1:A:292:ILE:HD13	1.75	0.68
3:L:68:GLY:O	3:L:69:THR:HB	1.94	0.66
1:A:40:ARG:HG2	1:A:283:PHE:HB3	1.78	0.65
2:H:47:TRP:HB2	3:L:95:LEU:HD22	1.79	0.65
3:D:12:SER:HA	3:D:104:GLU:O	1.96	0.65
3:D:24:LYS:CE	3:D:70:ASP:OD1	2.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:LEU:HD11	1:B:501:LEU:HD12	1.79	0.64
3:D:68:GLY:O	3:D:69:THR:HB	1.99	0.62
1:A:497:LEU:HD11	1:A:501:LEU:HD12	1.82	0.61
1:A:141:SER:O	1:A:142:ALA:HB3	2.01	0.59
2:C:37:VAL:HG12	2:C:47:TRP:HA	1.86	0.56
3:L:55:TYR:O	3:L:58:VAL:HG13	2.06	0.56
3:L:30:THR:HG22	3:L:31:ASN:N	2.13	0.56
1:A:175:GLY:HA2	1:A:218:LEU:O	2.05	0.55
1:B:497:LEU:CD1	1:B:501:LEU:HD12	2.36	0.55
1:A:508:PHE:HB3	1:A:511:ILE:HD12	1.89	0.54
1:A:497:LEU:CD1	1:A:501:LEU:HD12	2.38	0.54
3:L:2:ILE:HG12	3:L:27:GLN:HG2	1.91	0.53
1:A:238:VAL:HG21	1:A:292:ILE:CD1	2.38	0.53
3:D:15:VAL:HG23	3:D:105:ILE:HG21	1.89	0.53
2:C:68:VAL:CG2	2:C:83:LEU:HD13	2.38	0.53
1:B:117:ASN:HD22	1:B:220:HIS:CD2	2.27	0.53
1:B:508:PHE:HB3	1:B:511:ILE:HD12	1.91	0.53
3:D:33:VAL:HA	3:D:89:GLN:O	2.09	0.53
2:H:130:PRO:HD3	2:H:216:LYS:HE2	1.92	0.52
1:B:40:ARG:HG3	1:B:283:PHE:HB3	1.91	0.52
2:C:43:GLN:HG3	6:C:328:HOH:O	2.10	0.52
1:B:111:ASP:O	1:B:138:PRO:HD2	2.10	0.52
1:A:111:ASP:O	1:A:138:PRO:HD2	2.09	0.51
1:B:141:SER:O	1:B:142:ALA:CB	2.52	0.51
3:L:8:PRO:O	3:L:9:SER:HB3	2.11	0.51
1:B:290:LEU:HD21	1:B:292:ILE:HD11	1.92	0.51
1:B:226:ASP:OD2	1:B:241:GLY:HA3	2.11	0.51
3:L:30:THR:CG2	3:L:31:ASN:N	2.73	0.51
3:L:158:SER:HA	3:L:177:THR:O	2.10	0.50
2:C:68:VAL:HG23	2:C:83:LEU:HD13	1.92	0.50
1:A:38:HIS:HE1	1:A:118:HIS:CD2	2.30	0.50
1:B:342:THR:HB	1:B:406:ILE:HD11	1.94	0.50
3:L:124:LEU:HD23	3:L:182:LYS:HE3	1.95	0.49
3:D:78:LEU:HD11	3:D:103:LEU:HD21	1.95	0.48
1:B:461:LEU:HD11	1:B:548:HIS:ND1	2.29	0.48
3:L:78:LEU:HD11	3:L:103:LEU:HD21	1.95	0.47
1:A:472:LEU:HD23	1:A:487:LEU:HD22	1.97	0.47
1:A:231:GLN:HA	1:A:269:SER:HA	1.96	0.47
1:A:501:LEU:HD22	1:A:508:PHE:CD2	2.50	0.47
2:H:29:PHE:CD2	2:H:77:SER:HA	2.50	0.47
3:D:11:LEU:HD22	3:D:12:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:O	1:A:142:ALA:CB	2.63	0.46
1:B:197:ILE:HD11	1:B:228:LEU:HB3	1.98	0.46
1:B:501:LEU:HD22	1:B:508:PHE:CD2	2.50	0.46
2:C:7:SER:HB3	2:C:21:SER:H	1.80	0.46
1:A:435:PHE:O	1:A:438:SER:HB3	2.15	0.46
1:A:497:LEU:HD11	1:A:501:LEU:CD1	2.47	0.45
1:B:341:LYS:HA	1:B:404:GLY:O	2.16	0.45
2:H:11:VAL:HB	2:H:154:PRO:HG3	1.99	0.45
1:A:129:GLU:HA	1:A:130:PRO:HA	1.78	0.45
1:A:341:LYS:HA	1:A:404:GLY:O	2.17	0.45
1:B:294:PHE:HA	1:B:299:ASN:O	2.17	0.45
2:H:149:VAL:HG11	2:H:157:VAL:HG11	1.99	0.44
3:D:47:LEU:HA	3:D:58:VAL:HG21	1.99	0.44
1:B:64:LEU:HD11	1:B:287:LEU:HD13	1.98	0.44
3:L:33:VAL:HA	3:L:89:GLN:O	2.18	0.44
1:A:64:LEU:HD11	1:A:287:LEU:HD13	1.98	0.44
1:A:117:ASN:HD22	1:A:220:HIS:CD2	2.36	0.44
1:B:291:LYS:HD2	1:B:304:HIS:CE1	2.53	0.44
1:A:342:THR:HB	1:A:406:ILE:HD11	2.00	0.44
1:B:204:VAL:HG12	1:B:208:LYS:HE2	1.99	0.44
3:L:95:LEU:HD21	3:L:97:PHE:CE1	2.53	0.44
3:L:131:VAL:HG13	3:L:178:LEU:HB3	2.00	0.44
1:B:175:GLY:HA2	1:B:218:LEU:O	2.18	0.43
2:H:188:VAL:HG21	3:L:134:LEU:HD22	2.01	0.43
1:A:204:VAL:HG12	1:A:208:LYS:HE2	1.99	0.43
1:B:388:ILE:HG22	1:B:452:VAL:HG12	2.00	0.43
3:D:83:ILE:O	3:D:83:ILE:HG23	2.18	0.43
2:H:149:VAL:HB	2:H:185:LEU:HB3	2.01	0.43
1:B:497:LEU:HD11	1:B:501:LEU:CD1	2.45	0.43
3:L:105:ILE:HD11	3:L:170:SER:CB	2.49	0.43
2:C:30:ALA:HA	2:C:53:PRO:HB2	2.00	0.43
1:A:388:ILE:CG1	1:A:497:LEU:HD13	2.38	0.43
2:H:19:LYS:HG3	2:H:82:GLU:HB2	2.01	0.43
3:L:83:ILE:HG23	3:L:83:ILE:O	2.19	0.42
1:A:39:SER:OG	1:A:93:PHE:HB2	2.20	0.42
2:C:19:LYS:HG3	2:C:82:GLU:HB2	2.01	0.42
1:B:408:TRP:HZ3	1:B:525:ILE:HG12	1.83	0.42
3:L:118:PRO:HB3	3:L:208:PHE:CE2	2.54	0.42
2:H:18:VAL:O	2:H:82:GLU:HA	2.20	0.42
1:A:395:ARG:HB2	1:A:413:ALA:O	2.20	0.42
3:L:54:ARG:CG	3:L:58:VAL:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:THR:HG23	2:C:117:THR:HA	2.02	0.42
1:A:485:ASP:HB2	6:A:855:HOH:O	2.19	0.41
1:B:357:GLU:HB2	1:B:546:ILE:HB	2.01	0.41
1:B:82:ASP:HB2	1:B:110:TYR:CE2	2.55	0.41
1:B:388:ILE:CG1	1:B:497:LEU:HD13	2.38	0.41
1:A:388:ILE:HG22	1:A:452:VAL:HG12	2.02	0.41
2:C:18:VAL:O	2:C:82:GLU:HA	2.21	0.41
1:A:357:GLU:HB2	1:A:546:ILE:HB	2.03	0.41
2:C:98:ARG:NH1	2:C:99:GLY:O	2.54	0.41
2:H:37:VAL:HG12	2:H:47:TRP:HA	2.03	0.41
1:B:141:SER:O	1:B:175:GLY:O	2.39	0.41
1:B:380:PHE:HA	1:B:477:THR:O	2.20	0.41
3:D:37:GLN:HB2	3:D:47:LEU:HD11	2.03	0.40
3:L:135:LEU:HD22	3:L:174:LEU:HD23	2.04	0.40
1:B:35:ASN:HB3	1:B:83:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/527 (99%)	489 (94%)	29 (6%)	3 (1%)	22	48
1	B	521/527 (99%)	484 (93%)	35 (7%)	2 (0%)	30	58
2	C	211/231 (91%)	194 (92%)	14 (7%)	3 (1%)	9	27
2	H	211/231 (91%)	195 (92%)	12 (6%)	4 (2%)	6	20
3	D	207/209 (99%)	180 (87%)	16 (8%)	11 (5%)	1	4
3	L	207/209 (99%)	182 (88%)	18 (9%)	7 (3%)	3	9
All	All	1878/1934 (97%)	1724 (92%)	124 (7%)	30 (2%)	8	24

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	163	SER
3	D	40	PRO
3	D	150	ASP
3	D	165	GLN
3	D	167	SER
3	L	40	PRO
3	L	56	THR
3	L	69	THR
1	A	88	GLN
1	A	377	ASP
3	D	68	GLY
3	D	69	THR
3	D	137	ASN
3	L	68	GLY
3	L	137	ASN
2	C	67	ARG
3	D	142	GLU
3	D	166	ASP
1	A	337	GLN
2	C	2	ILE
3	L	158	SER
1	B	88	GLN
3	D	158	SER
2	H	2	ILE
2	H	178	GLN
2	H	198	THR
1	B	142	ALA
3	D	83	ILE
2	H	163	SER
3	L	83	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/455 (98%)	444 (99%)	4 (1%)	75	91
1	B	446/455 (98%)	444 (100%)	2 (0%)	89	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	180/195 (92%)	168 (93%)	12 (7%)	13	35
2	H	180/195 (92%)	171 (95%)	9 (5%)	20	48
3	D	185/185 (100%)	178 (96%)	7 (4%)	28	59
3	L	185/185 (100%)	175 (95%)	10 (5%)	18	45
All	All	1624/1670 (97%)	1580 (97%)	44 (3%)	40	71

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	117	ASN
1	A	365	CYS
1	A	506	ASP
1	B	228	LEU
1	B	487	LEU
2	C	63	LYS
2	C	72	ARG
2	C	81	MET
2	C	117	THR
2	C	142	THR
2	C	155	GLU
2	C	157	VAL
2	C	188	VAL
2	C	193	SER
2	C	200	THR
2	C	204	ASN
2	C	208	LYS
3	D	24	LYS
3	D	116	ILE
3	D	125	LYS
3	D	131	VAL
3	D	166	ASP
3	D	173	SER
3	D	205	THR
2	H	58	SER
2	H	72	ARG
2	H	122	SER
2	H	142	THR
2	H	155	GLU
2	H	188	VAL
2	H	193	SER

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Mol	Chain	Res	Type
2	H	200	THR
2	H	208	LYS
3	L	24	LYS
3	L	93	SER
3	L	105	ILE
3	L	116	ILE
3	L	125	LYS
3	L	131	VAL
3	L	150	ASP
3	L	167	SER
3	L	173	SER
3	L	205	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	GLN
1	B	304	HIS
1	B	549	HIS
3	D	53	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	601	1	14,14,15	0.32	0	17,19,21	0.77	2 (11%)
4	NAG	A	601	1	14,14,15	0.32	0	17,19,21	0.73	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	601	NAG	C1-O5-C5	2.12	115.06	112.19
4	B	601	NAG	O5-C1-C2	-2.11	107.96	111.29
4	A	601	NAG	O5-C1-C2	-2.09	107.99	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	523/527 (99%)	-0.32	3 (0%) 85 82	38, 54, 81, 120	0
1	B	523/527 (99%)	-0.35	3 (0%) 85 82	37, 53, 75, 118	0
2	C	119/231 (51%)	0.33	5 (4%) 41 36	53, 88, 122, 145	0
2	H	215/231 (93%)	0.07	13 (6%) 29 24	42, 62, 110, 145	0
3	D	104/209 (49%)	0.39	3 (2%) 54 48	53, 85, 122, 161	0
3	L	209/209 (100%)	0.18	7 (3%) 49 44	41, 71, 119, 136	0
All	All	1693/1934 (87%)	-0.13	34 (2%) 64 59	37, 57, 109, 161	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	105	ILE	6.4
2	H	164	GLY	4.6
2	H	165	ALA	4.0
1	B	549	HIS	3.9
1	A	334	TYR	3.6
2	C	119	SER	3.5
1	A	549	HIS	3.4
3	L	125	LYS	3.2
2	H	135	SER	2.8
3	D	103	LEU	2.8
2	H	197	GLY	2.8
2	C	81	MET	2.7
2	H	142	THR	2.6
1	B	375	HIS	2.5
3	L	152	ALA	2.5
2	H	201	TYR	2.5
3	L	126	SER	2.4
2	H	218	VAL	2.4
2	H	199	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	375	HIS	2.4
2	H	131	LEU	2.3
2	H	134	SER	2.3
2	C	37	VAL	2.3
3	L	124	LEU	2.3
3	L	191	TYR	2.2
2	C	47	TRP	2.2
3	L	128	THR	2.2
2	H	214	VAL	2.2
2	H	219	GLU	2.1
3	L	148	LYS	2.1
2	H	163	SER	2.1
2	C	24	ALA	2.1
3	D	62	PHE	2.0
1	B	333	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	601	14/15	0.86	0.12	90,96,99,99	0
4	NAG	B	601	14/15	0.88	0.10	72,77,81,82	0
5	ZN	A	603	1/1	0.96	0.11	74,74,74,74	0
5	ZN	A	602	1/1	0.97	0.10	56,56,56,56	0
5	ZN	B	602	1/1	0.98	0.10	51,51,51,51	0
5	ZN	B	603	1/1	0.98	0.09	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.